



Subject card

Subject name and code	Information technology, PG_00053223						
Field of study	Chemistry						
Date of commencement of studies	October 2022	Academic year of realisation of subject				2022/2023	
Education level	first-cycle studies	Subject group			Obligatory subject group in the field of study		
Mode of study	Full-time studies	Mode of delivery			at the university		
Year of study	1	Language of instruction			Polish		
Semester of study	1	ECTS credits			5.0		
Learning profile	general academic profile	Assessment form			assessment		
Conducting unit	Department of Analytical Chemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Dorota Warmińska				
	Teachers		dr hab. inż. Dorota Warmińska dr inż. Anna Kuffel Joanna Słabońska dr inż. Mateusz Kogut mgr inż. Bartosz Nowosielski				
Lesson type and method of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	15.0	45.0	0.0	0.0	75
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours		Self-study	SUM	
	Number of study hours	75	5.0		45.0	125	
Subject objectives	The aim of the course is to familiarize students with the possibilities offered by modern personal computer software in the field of calculation and text editing. In addition, the aim of the course is to develop the student's ability to use the computer for statistical and numerical analysis of a set of a chemical experiment results.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[K6_W05] knows and understands the chemical processes and algorithms of mathematical models which are necessary for the design of technological processes, knows chemical structure of contemporary materials and its relation to their properties, enabling the selection of the materials for sustainable development technology and material-efficient and energy-efficient methods		The student knows and is able to use mathematical models necessary to design technological processes		[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge		
	[K6_U03] can make detailed documentation of the results of self-conducted experiments and prepare a report describing these results		After completing the course, the student should be able to prepare the elaboration of the obtained results, fluently using the advanced functions of MS Office programs (Word, Excel).		[SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment		
	[K6_U05] can, on the basis of the collected experimental or source material, prepare an oral communication with a multimedia presentation		The student is able to prepare and present a speech along with the presentation of the results using appropriately selected computer programs		[SU5] Assessment of ability to present the results of task [SU1] Assessment of task fulfilment		

Subject contents	<p>Laboratory:</p> <p>Working principles in the Windows operating system: local area network, information organization, transfer data between applications. Web browser support, principles of searching for information on the web, search engines, databases, chemical data resources on the Internet. Using the Word editor to prepare chemistry texts: using the equation editor, preparing tabular summaries in a text editor, combining text with graphic elements. Application of Excel spreadsheet for presentation and solving chemical problems. Basic calculations in the spreadsheet, priorities of activities, use of functions embedded, formatting calculation results. Ways of addressing cells and their consequences. Rules for using cell names, areas and formulas. Drawing up graphs: presentation dependencies described by the formula and tabular data, trend lines, scale change on the chart axes. Preparation of an example presentation using the Power Point program. Solving nonlinear equations. Linear regression, linearization of nonlinear dependencies, multiple regression. Numerical integration.</p> <p>Exercises:</p> <p>Evaluation of the correctness of experimental data. Estimating the size of errors. Analysis of results of one-dimensional random variable. Calculation of the mean, median, variance. Determination of the confidence interval. Conducting statistical tests. Analysis of a two-dimensional random variable. Regression and correlation study. Determination of linear and nonlinear regression parameters. Solving nonlinear equations by numerical methods. Interpolation. Numerical calculation of the definite integral.</p> <p>Lectures:</p> <p>Basic concepts of error theory, sources of errors. The difference between concepts: uncertainty and error. Systematic and random errors. Maximum error, probability and error propagation and rounding rules. One-dimensional random variable. Measures of location and dispersion. Normal distribution and t Student (mean and its confidence interval, median and fashion, gross error and its elimination, precision and accuracy, Q-Dixon, F-Snedecor and Student t-tests) Two-dimensional random variable. Regression and correlation. Linear, nonlinear and multiple regression. Residual distribution, residual variance. Regression coefficient confidence interval. Tolerance range for values deviating from the regression line. Stages of IT development. Algorithm, algorithm features, construction principles, typical structures of activity networks. Algorithm stability. Examples of numerical instability. Solving nonlinear and leap equations using bisection, tangent, secant and straight iteration methods. Interpolation and differentiation of a tabular function (Newton's formulas based on finite differences and differential quotients of a function, Lagrange's formula). Numerical integration (Newton-Cotes formulas, generalized trapezoidal formulas, parabolas, Richardson extrapolation).</p>														
Prerequisites and co-requisites															
Assessment methods and criteria	<table border="1"> <thead> <tr> <th data-bbox="456 1245 794 1272">Subject passing criteria</th> <th data-bbox="799 1245 1137 1272">Passing threshold</th> <th data-bbox="1142 1245 1481 1272">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="456 1279 794 1328">Lecter - Colloquia during the semester</td> <td data-bbox="799 1279 1137 1328">50.0%</td> <td data-bbox="1142 1279 1481 1328">30.0%</td> </tr> <tr> <td data-bbox="456 1335 794 1384">Classes-Colloquia during the semester</td> <td data-bbox="799 1335 1137 1384">50.0%</td> <td data-bbox="1142 1335 1481 1384">30.0%</td> </tr> <tr> <td data-bbox="456 1391 794 1440">Laboratory-Colloquia during the semester</td> <td data-bbox="799 1391 1137 1440">50.0%</td> <td data-bbox="1142 1391 1481 1440">40.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	Lecter - Colloquia during the semester	50.0%	30.0%	Classes-Colloquia during the semester	50.0%	30.0%	Laboratory-Colloquia during the semester	50.0%	40.0%
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Recommended reading	<p>Basic literature</p> <p>J.B. Czerwiński i inni, Metody statystyczne dla chemików PWN 1986</p> <p>K. Doerffel, Statystyka dla chemików analityków, WNT 1989</p> <p>J. Arendarski, Niepewność pomiarów, Politechnika Warszawska, 2003</p> <p>T. Ratajczak, Metody numeryczne przykłady i zadania, Wydawnictwo PG, Gdańsk 2007</p> <p>E. Slavicek, Technika obliczeniowa dla chemików WNT 1991</p>														

	Supplementary literature	<p>P. Konieczka, J. Namieśnik i inni, Ocena i kontrola jakości wyników pomiarów analitycznych, WNT Warszawa 2007</p> <p>E. Bulska i inni, Ocena i kontrola jakości wyników pomiarów analitycznych, WNT 2007</p> <p>Z. Fortuna, B. Macukow, J. Wąsowski, Metody numeryczne, WNT wznawiane każdego roku.</p> <p>A. Bjork, G. Dahlquist, Metody numeryczne PWN 1987</p>
	eResources addresses	
Example issues/ example questions/ tasks being completed	<p>Creating a network of simple algorithms for computational methods.</p> <p>Determining the confidence interval for the arithmetic mean of the experimental data set.</p> <p>Performing conformity assessment of the accuracy and precision of the measurement method</p> <p>Calculation of the optimal regression line.</p> <p>Preparation of an example presentation using the Power Point program.</p>	
Work placement	Not applicable	